Scientists use world's fastest computer to model materials under extreme conditions

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Advances in experimental techniques and supercomputer performance, culminating with Roadrunner, have reduced the gap between experiment and simulation

Los Alamos, New Mexico, October 30, 2009—The long-established and reliable SPaSM (Scalable Parallel Short-range Molecular dynamics) code, adapted to run on the world's fastest supercomputer, Roadrunner, is being used to study the physics of how materials break up, called "spall," and how pieces fly off, called "ejecta," from thin sheets of copper as shock waves force the material break apart at the atomic scale.Because of

Roadrunner's unique capability, materials scientists are for the first time attempting to create atomic-scale models that describe how voids are created, grow, and merge; how materials may swell or shrink under stress; and how once broken bonds might reattach, and they're doing it at size and time scales that approach those of actual experiments, so that the models can be validated experimentally. "One of the interests we have had is looking at shock waves in metals and how the metals deform, they may melt under shock loading or change their crystalline structure," said Tim Germann of the Physics and Chemistry of Materials (T-1) group. "Our multibillion-atom molecular dynamics code is providing unprecedented insight into the nature of the critical event controlling the strength of materials, a fundamental long-standing problem in materials science."In the past, there has been a distinct gap between the microscopic, ultrafast processes that could be studied by molecular dynamics simulations, and the usual engineering-scale behavior of shock experiments.

For instance, gas gun experiments launch a "flyer plate" impactor at a target sample whose thickness is typically several millimeters, while simulations struggled to reach hundreds of nanometers, 4 orders of magnitude smaller in size. (And similarly in time; the corresponding shock transit times in such experiments are microseconds, and tens to hundreds of picoseconds in simulations.) Some phenomena, such as the nucleation, growth, and coalescence of voids following shock compression and release, which can lead to "spall failure" as the material breaks apart, take place at precisely the time and length scales which were inaccessible to both simulation and experiment, and thus have typically been described by "trial and error" models which could never be directly verified. However, steady advances by both experimental techniques, including laser-driven shock waves in thin metal foils using ultrafast X-ray diffraction to monitor structural changes, and in simulation techniques and supercomputer performance, culminating with Roadrunner, have closed this gap and are now enabling both simulations and experiments to probe shock deformation at similar length, 1-10 microns, and nanosecond time scales.Spall failure and the ejection of material from shocked metal surfaces are problems that have attracted increased attention both experimentally and theoretically at Los Alamos. Models are required that can predict both when a material will fail, and the amount of mass ejected from a shocked interface with a given surface finish and strength."We've already created simulations with quasi-two dimensional geometries that have helped explain the production of ejecta in the first nanosecond after a shock," said Germann. "The Roadrunner simulations are aimed at understanding later effects like jet breakup and three dimensional droplet formation, including the resultant particle sizes, velocities and the relationship between the two." About Roadrunner, the world's fastest supercomputer, first to break the petaflop barrierOn Memorial Day, May 26, 2008, the "Roadrunner" supercomputer exceeded a sustained speed of 1 petaflop/s, or 1 million billion calculations per second. "Petaflop/s" is computer jargon—peta signifying the number 1 followed by 15 zeros (sometimes called a quadrillion) and flop/s meaning "floating point operation per second." Shortly after that it was named the world's fastest supercomputer by the TOP500 organization at the June 2008 International Supercomputing Conference in Dresden Germany.The Roadrunner supercomputer, developed by IBM in partnership with the Laboratory and the National Nuclear Security Administration, will be used to perform advanced physics and predictive simulations in a classified mode to assure the safety, security, and reliability of the U.S. nuclear deterrent. The system will be used by scientists at the NNSA's Los Alamos, Sandia, and Lawrence Livermore national laboratories.The secret to its record-breaking performance is a unique hybrid design. Each compute node in this cluster consists of two AMD Opteron™ dual-core processors plus four PowerXCell 8i™ processors used as computational accelerators. The accelerators used in Roadrunner are a special IBM-developed variant of the Cell processor used in the Sony PlayStation 3®. The node-attached Cell accelerators are what make Roadrunner different than typical clusters.Roadrunner is still currently the world's fastest with a speed of 1.105 petaflop/s per second, according to the TOP500 announcement at the November 2008 Supercomputing Conference in Austin Texas, and itagain retained the #1 position at the June ISC09 conference.

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